

members, NUGEX, and PNNL-ASGC division

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Background & short history of WRF-SIG

- Discussions in NUGEX monthly meetings early this year (2022)
 "How NUG members can benefit both the individual and community"
 - (Pieter Maris will present more in the later session)
- One of the ideas "Topic-based subgroups of NUG with supporting infrastructure"
 Example topics: ML, MPI, OpenMP, Fortran, VASP, climate models, Python, PSC, ORNL, grad students
- Picked the WRF model used in the climate science community as a pilot topic
- Modest advertisement in May-June
 - NERSC weekly email, NUG monthly meeting, and a few email lists among DOE SC Earth and Environmental Systems Sciences Division (EESSD)
- Google form to register for the email list
- Currently ~30 members registered

Members from DOE labs, Universities, NERSC User support, industry/consulting Graduate students, early-mid career scientists/faculties

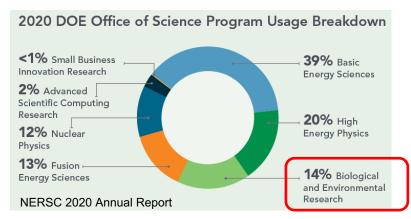


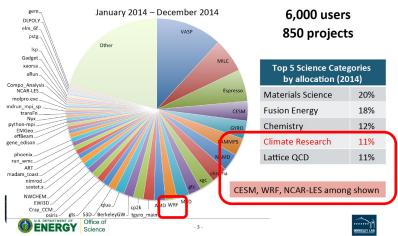






Motivation for the SIG #1: many WRF users at NERSC





70 Climate Projects at NERSC (AY2016)



- Awards are published at:
 - https://www.nersc.gov/users/accounts/awardedprojects/2016-allocation-awards/
- See the detailed list of projects in "Extra Slides" (ordered by allocation hours).
- 30 projects use CESM/ACME or CESM components.
 254 active users
- 17 projects use WRF. 85 users (36 active).

"Climate Applications Support at NERSC" (Helen He, 2016)

~40-50 active WRF users from ~ 20 projects



Possible >20 duplications of tickets and standard input data





What is the Weather Research Forecasting (WRF) model?

Numerical model to integrate coupled partial differential equations of the dynamics of the atmosphere:

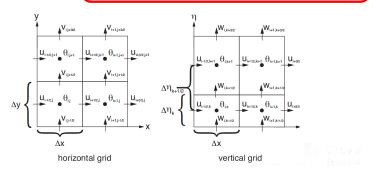
- Conservation of momentum & mass (AKA Navier-Stokes equations),
- Conservation of energy (first law of thermodynamics)
- Conservation of other trace constituents in the atmosphere (e.g., aerosol, cloud droplets)

with appropriate approximations for the Earth's atmosphere

$$\frac{\partial \bar{\rho} \mathbf{u}}{\partial t} = -\nabla \cdot (\bar{\rho} \mathbf{u} \mathbf{u}) - \nabla p + \dots + S_d + S_p$$

$$S_d : \text{unresolved dynamics}$$

$$S_p : \text{radiative, chemical, and many other processes}$$



Equations are discretized on a Cartesian grid with a finite resolution

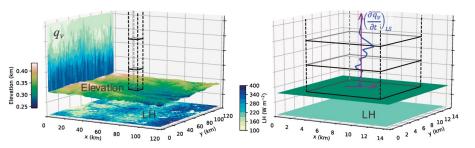
Skamarock et al., 2019, WRF-ARW v4

doi:10.5065/1dfh-6p97

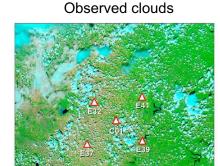
- Includes statistical/empirical/theoretical models to predict upscale effects from unresolved air motions
- Includes statistical/empirical/theoretical models to predict processes not included in the above equations (e.g., radiative transfer, chemical reactions, land surface ecology, etc.)
- Two main variants; one for weather forecast, and the other for academic research: "Advanced Research WRF (ARW)"
- Developed by science communities and maintained by the Mesoscale & Microscale Meteorology Laboratory at the National Center for Atmospheric Research BERKELEY LAB

AR WRF applications

Realistic and idealized simulations for process understanding



(Ovchinnikov et al. 2022)



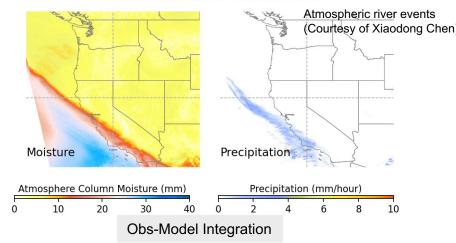
Simulated clouds

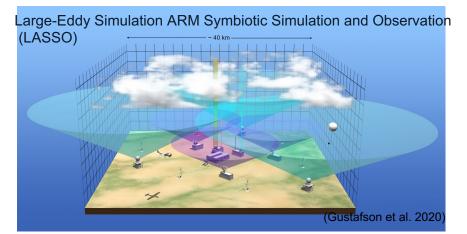


(Fast et al. 2019)

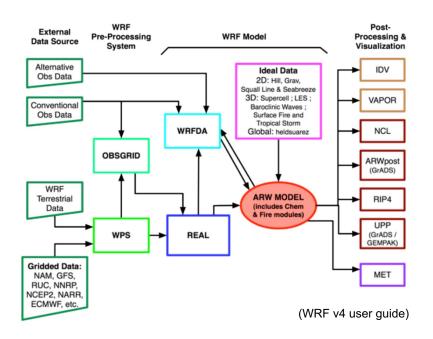
Climate simulations, extreme events

Time: 1997-01-15 01:00:00 UTC





WRF software



Language

Model code: Fortran Ancillary programs: C

Build system: perl, make, C & Bourne shell

Parallelism

"The WRF model may be built to run on a single-processor machine, a shared-memory machine (that uses the **OpenMP API**), a distributed memory machine (with the appropriate **MPI libraries**), or on a distributed cluster (utilizing both OpenMP and MPI). "

Main dependencies are mostly I/O

NETCDF (& HDF5), parallel netcdf, jasper, png, zlib Most of them available as modules at NERSC

A wide range of applications and target scales, making the model code very complex











Motivation for the SIG #2: many WRF users experience challenges

Feedback from the WRF-SIG early members in the first virtual meeting

- Difficult to compile HPC system and general documentation are complex
- Simulation is slow, and queue wait time is long
- Another HPC center has common input data on the system

Possible Reasons & where we can improve

Lack of documentation & examples with specifics of WRF + NERSC

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(e.g., cross-compilation for KNL, compiler selection/options, dependent modules) (general documentation may not be understood by domain-scientists, especially students)
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Lack of communication channels among WRF users at NERSC

(a solution to a problem not efficiently shared among NERSC WRF users)









How we address the challenges through WRF-SIG

1. WRF at NERSC webpage in the official NERSC documentation

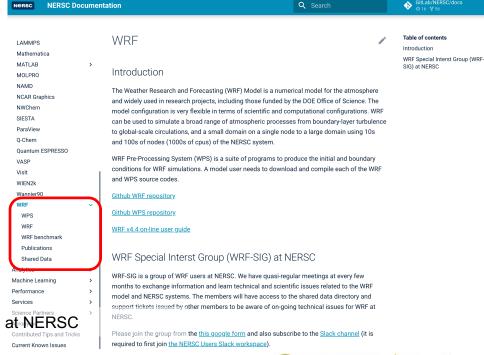
Working on draft webpage

Consider a wide range of readers:

- Graduate students / post-docs without software engineering/HPC training
- Non-native English speakers

Topics:

- Parallel programing options in WRF/ which option to select for a given WRF use case on NERSC systems
- Example scripts
- List of peer-reviewed papers using WRF at NERSC
- List of publicly available data generated for/by WRF at NERSC













How we address the challenges through WRF-SIG

2. Project account with small computing hours and storage allocation for SIG

- When a member issues a **service ticket**, other members can view and search for the ticket
- Small node hours for benchmark simulations, best-practice tests for documentation, and occasional test simulations after system updates
- CFS storage for common input data (e.g., global topography, land surface characteristics) and shared code/scripts

Submitted an ERCAP request for this year (2022)

★ Project Title
 The Weather Research and Forecasting (WRF) Model Special Interest Group
 ★ Label

WRF-SIG

2,000 cpu node hours, 1TB CFS storage











How we address the challenges through WRF-SIG

3. Quasi-regular virtual meetings and Slack channel

1st meeting in May, 2nd meeting in August, ~ 10 members attend each

Topics discussed:

Difficulties to compile and run WRF
Resources needed to increase productivity
Future of the WRF model and alternatives
(no official plans to port WRF to GPU systems)

WRF at NERSC webpage topics
WRF compilation workflow for Cori
Modules for WRF dependent libraries
Compiler wrappers

Perlmutter environment
WRF performance on NERS systems
(e.g., pure MPI vs. OpenMP + MPI)

Future meeting topics

Slack channel in the NERSC Users Slack workspace

16 members registered Not very active yet



Once the SIG gets allocation and the documentation webpage starts, we will use the Slack channel to share service tickets, test simulation results, updates on shared data & documentation, etc.









WRF-SIG summary

- Pilot special interest group initiated from discussions in NUGEX meetings
- Identified user needs for systematic and community-based support to boost productivity using the WRF model at NERSC
- Slow but steady progress (volunteer-based) :
 - 1. Drafting the WRF at NERSC webpages in the official NERSC documentation
 - 2. Applied for small computing hours and storage allocation for the group
 - 3. Started quasi-regular virtual meetings and Slack channel
- Lessens learned:
 - Google form is better than spreadsheet
 - Set the meeting reminder for the meeting calendar invite
 - Registration (Google) form should ask for which project accounts the user runs WRF this information helps the ERCAP request







